

7,7'-(Carbonyldiimino)bis[4-hydroxy-2-naphthalenesulfonic acid]
134-47-4 | DTXSID7059642

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.86e-09 mmHg

Global applicability domain: Outside

Local applicability domain index: 1.04e-01

Confidence level: 3.61e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Ethoxysulfuron</div> <div>Measured: 1.65e-07</div> <div>Predicted: 5.60e-08</div>	<div>Image not found</div> <div>9,10-Anthracenedione, 1,4-bis(methylamino)-</div> <div>Measured: 1.80e-08</div> <div>Predicted: 4.57e-11</div>	<div>Image not found</div> <div>Cyprodinil</div> <div>Measured: 1.13e-08</div> <div>Predicted: 1.18e-06</div>
<div>Image not found</div> <div>1-Isobutoxypropan-2-ol</div> <div>Measured: 7.13e-08</div> <div>Predicted: 1.69</div>	<div>Image not found</div> <div>Cloxyfonac [ISO]</div> <div>Measured: 6.86e-12</div> <div>Predicted: 3.84e-07</div>	